Disulfoton 298-04-4 | DTXSID0022018

Model Performance

Model	Data	

Weighted KNN model

5-fold CV (75%)		Training (Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.87	0.81	0.87	0.82	0.86	0.86	

Model Results

Predicted value: 9.03e-05 mol/L

Global applicability domain: Inside

Local applicability domain index: 7.87e-01

Confidence level: 6.36e-01

Nearest Neighbors from the Training Set

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Disulfoton

Measured: 5.94e-05 Predicted: 9.03e-05

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Terbufos

Measured: 1.76e-05 Predicted: 3.85e-05

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Phorate

Measured: 1.92e-04 Predicted: 1.94e-04

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Isothioate

Measured: 3.73e-04 Predicted: 2.34e-04

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Thiometon

Measured: 8.12e-04 Predicted: 3.57e-04